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Stable Discretization of Time-Domain Solvers

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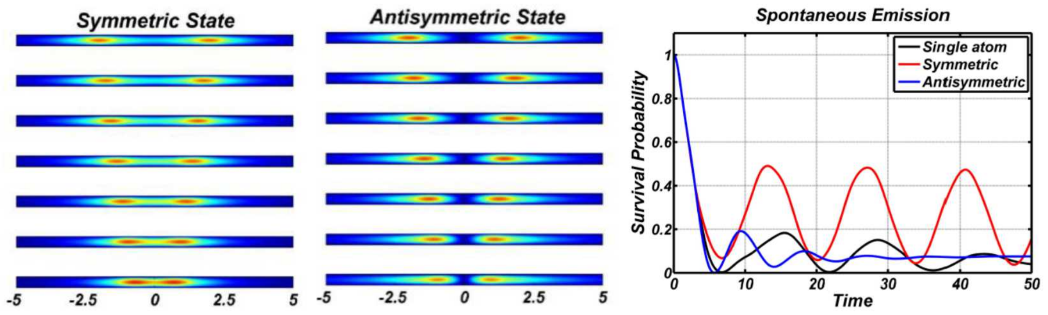
Introduction

- Emerging quantum physics applications stress the capabilities of currently available CEM tools
- To address some of the needs of this challenging new area, potential-based time domain integral equations (TDIEs) are being developed
- Initial work on potential-based TDIEs showed a profound connection between the basis functions used and the stability of the marching-on-in-time (MOT) method
  - Significantly more sensitive to choice of basis function than traditional field-based formulations
- Found that a previously developed functional framework could be used to rigorously determine appropriate potential-based TDIEs and basis functions to arrive at a stable MOT system
  - Functional framework is used to determine Sobolev spaces that act as domain and range for the relevant space-time integral operators
- Numerical results demonstrating the interesting sensitivity to Sobolev space properties of the potential-based TDIEs are shown

Quantum Physics & CEM

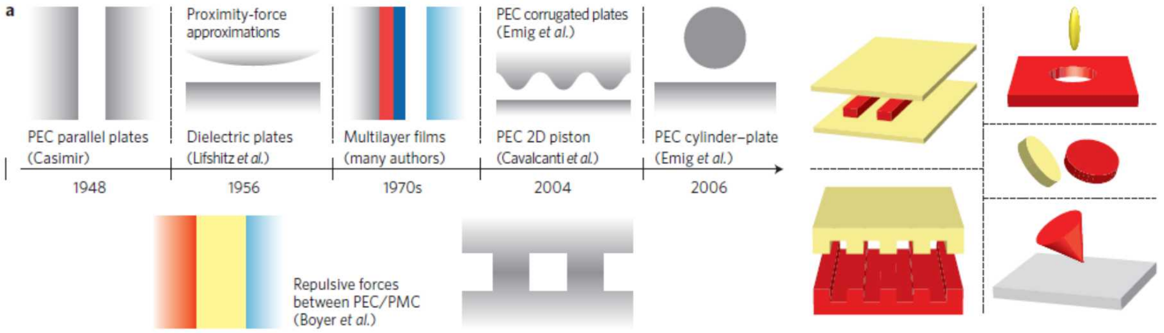
- Design of emerging quantum technologies will greatly benefit from improved *classical* CEM tools
- Large bandwidth requirements of many calculations make time domain methods appealing
- Time domain integral equation methods are of interest to efficiently analyze large systems of practical interest
  - Numerical stability from very low to high frequencies for multiscale or subwavelength geometries is needed – *challenging for traditional field-based methods (e.g., EFIE)*

Waveguide-QED



W. C. Chew, DOI: 10.1109/PIERS.2017.8262143

Casimir Force



F. Capasso, DOI: 10.1038/NPHOTON.2011.39

Emerging quantum applications require *classical* CEM tools for *increasingly* broadband analysis of multiscale, subwavelength, and lossy dielectrics

Potential-Based CEM

- Maxwell's equations are valid over vast length scales and broad frequency range
  - Subatomic to galactic; static to ultraviolet
  - Valid in quantum regime
- Discretized equations typically are not!
- Field-based formulation
  - Breaks down for low frequency or long wavelength
  - Not multiscale
- Potential-based formulation
  - Reinterpretation of how to solve Maxwell's equations numerically
  - Discrete equations do not break down
  - Good for analyzing multiscale/subwavelength structures
  - Potentials are typically quantities of interest for quantum applications

Field-based Formulation

Non-unique solution as $\omega \rightarrow 0$

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k^2\mathbf{E}(\mathbf{r}) = i\omega\mu\mathbf{J}(\mathbf{r}) - \nabla \times \mathbf{M}(\mathbf{r})$$

$$\nabla \times \nabla \times \mathbf{H}(\mathbf{r}) - k^2\mathbf{H}(\mathbf{r}) = i\omega\epsilon\mathbf{M}(\mathbf{r}) + \nabla \times \mathbf{J}(\mathbf{r})$$

Potential-based Formulation

No break down as $\omega \rightarrow 0$

$$\nabla^2\mathbf{A}(\mathbf{r}) + k^2\mathbf{A}(\mathbf{r}) = -\mu\mathbf{J}(\mathbf{r})$$

$$\nabla^2\Phi(\mathbf{r}) + k^2\Phi(\mathbf{r}) = -\rho(\mathbf{r})/\epsilon$$

Potential-Based CEM

- Potential-based TDIEs have been derived and shown to be stable for PEC objects
  - Equations have been a useful case study to investigate core aspects of stability of MOT discretized TDIEs
- Resulting systems perform well over broad frequency range, including very low frequencies
  - **A** equation captures quasi-magnetostatic physics
  - Φ equation captures quasi-electrostatic physics
  - Equations naturally decouple as frequency lowers, maintaining performance
- *Unknowns and equations are carefully selected based on a previously established rigorous functional framework for retarded potential boundary integral equations (DOI: 10.1007/978-3-642-55483-4_8)*

Differentiated A-Φ Integral Equations (D-APIE)

$$\hat{n}\times\int_S\left[\mu\frac{\dot{\mathbf{J}}(\mathbf{r}',t-R/c)}{4\pi R}-\nabla\frac{\Pi(\mathbf{r}',t-R/c)}{4\pi R}\right]dS'=\dot{\mathbf{A}}^{\text{inc}}(\mathbf{r},t)\times\hat{n}$$

$$\int_S\left[\epsilon^{-1}\frac{\nabla'\cdot\mathbf{J}(\mathbf{r}',t-R/c)}{4\pi R}-\frac{\dot{\Pi}(\mathbf{r}',t-R/c)}{4\pi R}\right]dS'=\dot{\Phi}^{\text{inc}}(\mathbf{r},t)$$

Unknowns: $\mathbf{J}(\mathbf{r}',t),\ \Pi(\mathbf{r}',t)=\hat{n}'\cdot\dot{\mathbf{A}}(\mathbf{r}',t)$

A-Φ Integral Equations (APIE)

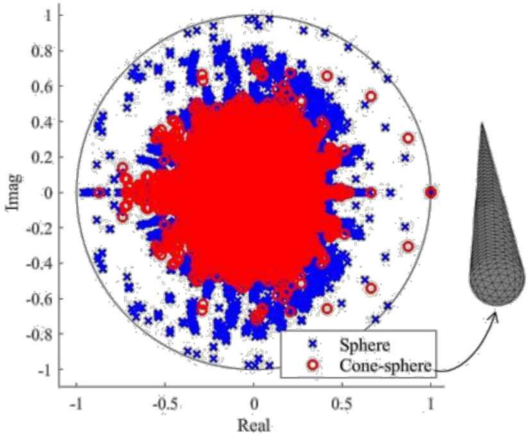
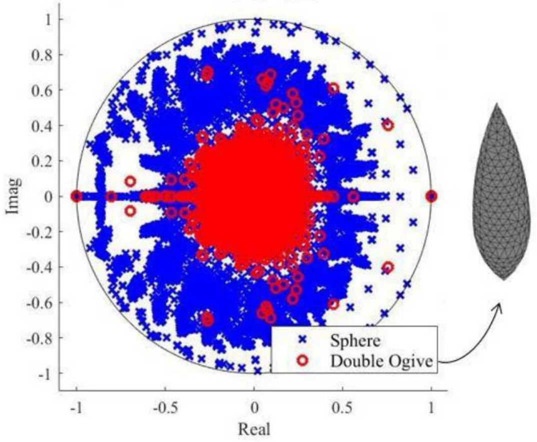
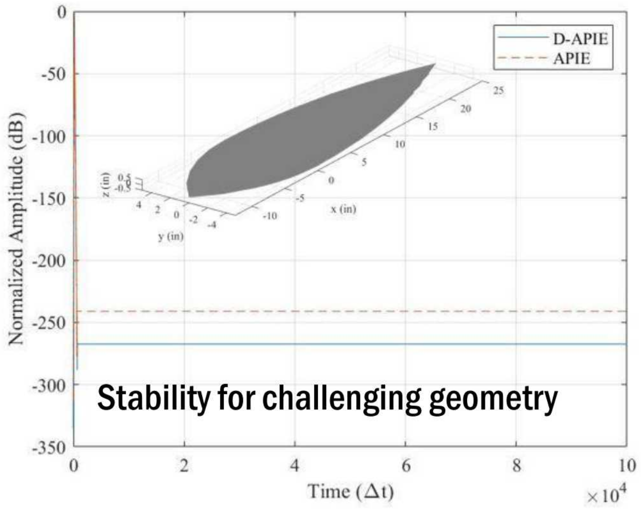
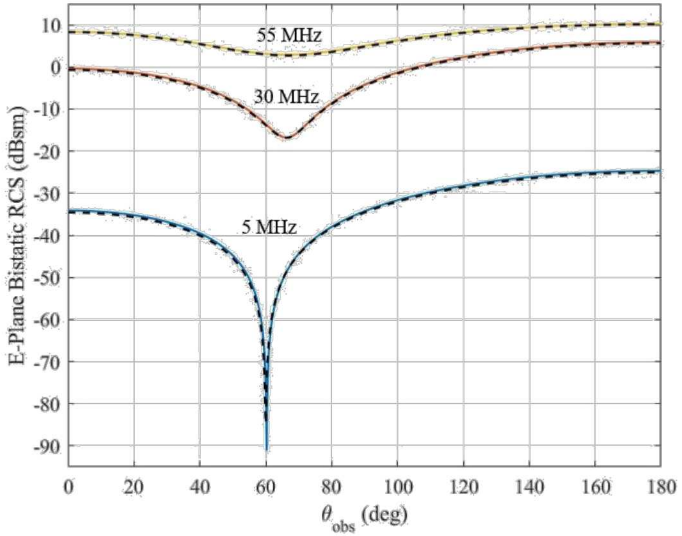
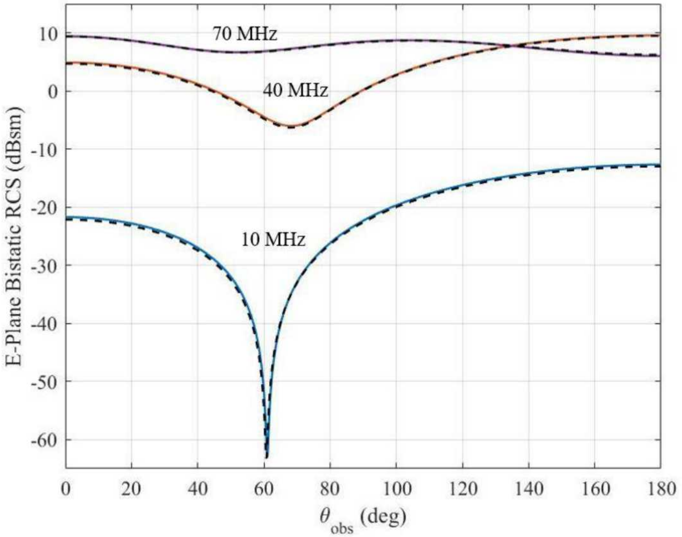
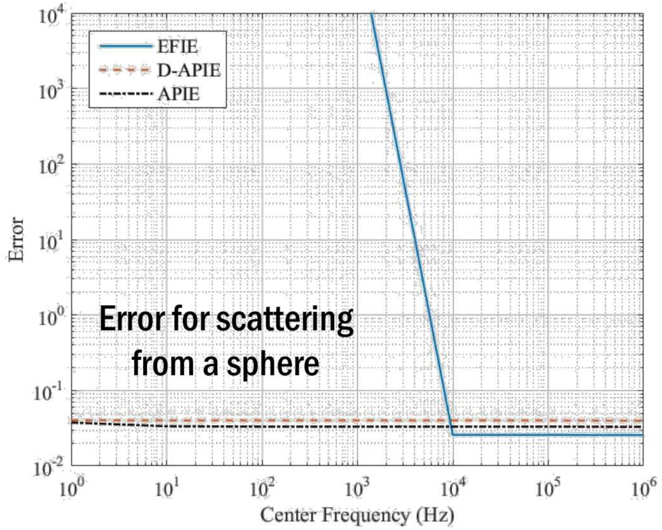
$$\hat{n}\times\int_S\left[\mu\frac{\mathbf{J}(\mathbf{r}',t-R/c)}{4\pi R}-\nabla\int_{-\infty}^{t-R/c}\frac{\Pi(\mathbf{r}',t')}{4\pi R}dt'\right]dS'=\mathbf{A}^{\text{inc}}(\mathbf{r},t)\times\hat{n}$$

$$\int_S\left[\epsilon^{-1}\int_{-\infty}^{t-R/c}\frac{\nabla'\cdot\mathbf{J}(\mathbf{r}',t')}{4\pi R}dt'-\frac{\Pi(\mathbf{r}',t-R/c)}{4\pi R}\right]dS'=\Phi^{\text{inc}}(\mathbf{r},t)$$

Unknowns: $\mathbf{J}(\mathbf{r}',t),\ \Pi(\mathbf{r}',t)=\hat{n}'\cdot\dot{\mathbf{A}}(\mathbf{r}',t)$

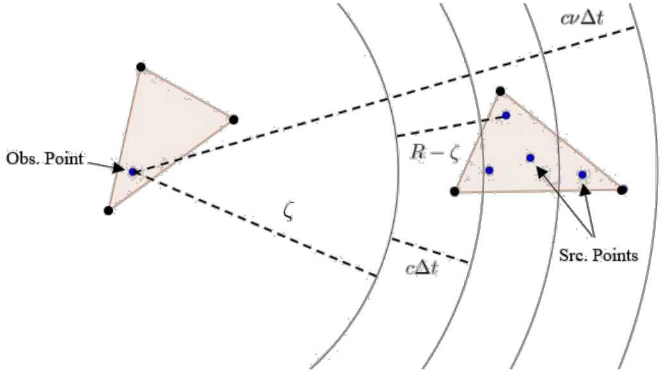
T. Roth, DOI: 10.1109/JMMCT.2018.2889535

Potential-Based CEM

	D-APIE	APIE	
Stability			
Accuracy			

Stability – A Closer Look

- Necessary (but not sufficient) condition for stability is to employ accurate numerical integration techniques
  - Integration is complicated due to the "shadowing" (incoming pulse doesn't always fully cover the spatial integration support)
- Two classes of techniques exist to evaluate the space-time integrals: quasi-exact/analytical and fully numerical methods
- Quasi-exact/analytical methods:
  - Applies only to RWG basis functions
  - B. Shanker, E. Michielssen, *et al.*, DOI: 10.1109 TAP.2009.2016700
  - A. Ergin, *et al.*, DOI: 10.1109/TAP.2011.2164180
- Separable expansion of Green's function (fully numerical technique):
  - Can be applied to arbitrary basis functions
  - B. Shanker, *et al.*, DOI: 10.1109/TAP.2012.220101



$$
\begin{aligned}
g(\mathbf{r},\mathbf{r}',t) &= \frac{1}{4\pi R}\delta(t-\zeta/c) * \delta(t-(R-\zeta)/c) \\
&= \frac{1}{4\pi R}\delta(t-\zeta/c) * \boxed{\sum_{l=0}^{\infty} a_l P_l(bt-1) P_l(\tilde{R})} \\
&\approx \frac{1}{4\pi R}\delta(t-\zeta/c) * \sum_{l=0}^{N_h} a_l P_l(bt-1) P_l(\tilde{R})
\end{aligned}
$$

Legendre polynomial completeness relation

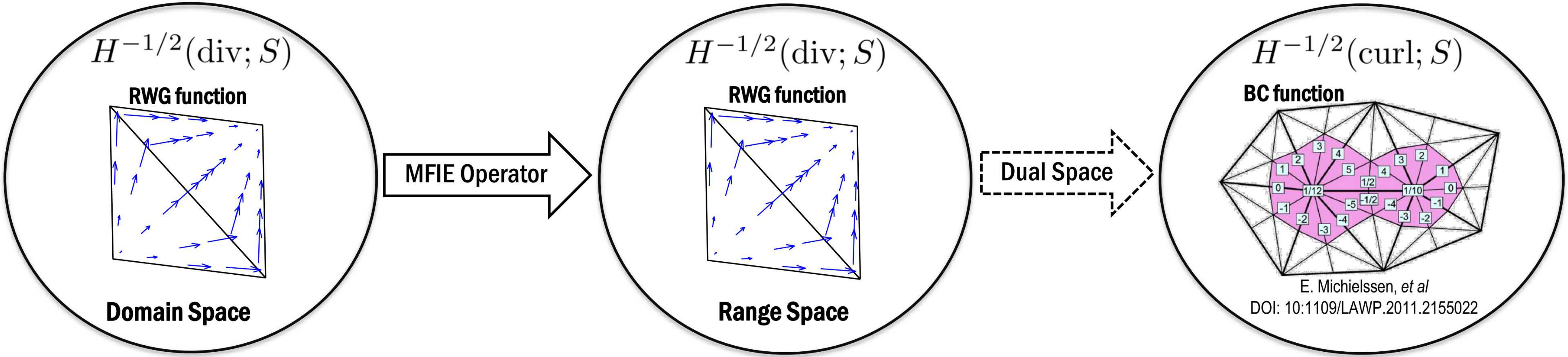
$$b = 2/(\nu\Delta t)$$

$$a_l = b(2l+1)/2$$

$$\tilde{R} = b(R-\zeta)/c - 1$$

Stability – A Closer Look

- Well known from frequency domain integral equations that the spatial discretization should conform to the Sobolev space properties of the operators for highest accuracy
  - Basis functions should be selected from domain space of the integral operator
  - Testing functions should be selected from dual space to the range of the integral operator



Less well known – temporal basis and testing functions should also conform to Sobolev space properties of the operator!

Stability – A Closer Look

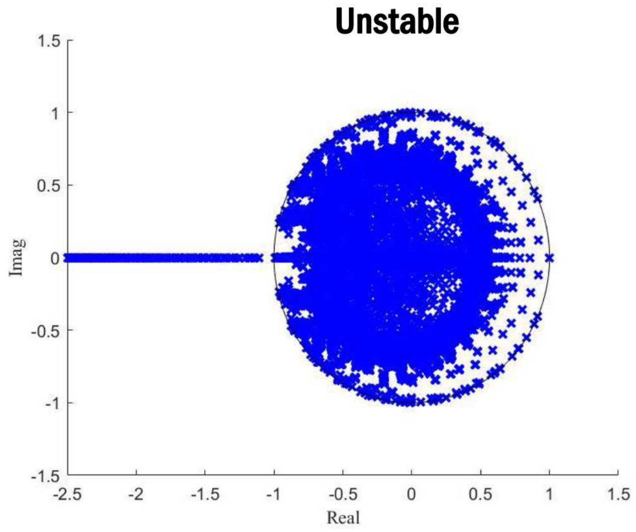
- Practical stability of MOT discretized TDIEs is substantially improved if temporal basis and testing functions are selected from correct temporal Sobolev space
  - Basis functions are selected from the domain of the integral operator
  - Testing functions are selected from the dual space to the range of the integral operator
- How to find temporal Sobolev spaces for space-time integral operators?
  - Ad hoc Sobolev spaces have been developed in the mathematical literature for exactly this purpose!
    - Review papers' DOIs: 10.1007/978-3-642-55483-4_8, 10.1007/s002110100251 (in French)

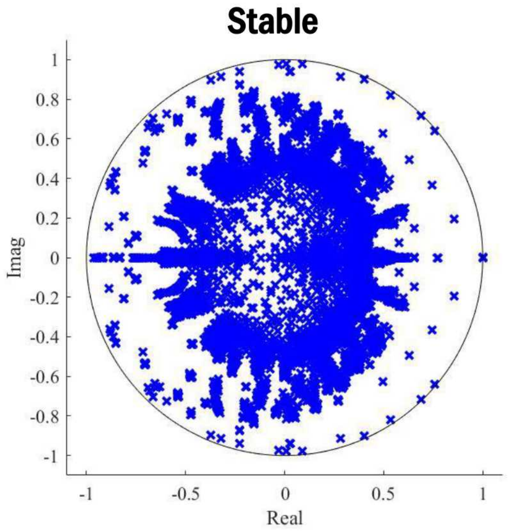
Steps to Determine Temporal Sobolev Spaces

1. Relate scattered EM energy in the time domain to the scattered EM energy in the frequency domain (Parseval's theorem)
2. Properties of the frequency domain integral operator are used to bound the scattered energy by the norm of the source function that produces the scattered field
   - *Determine domain space from this step*
3. Bound the norm of the source function by the energy of the incident field using properties of the integral equation and corresponding PDE
   - *Determine range space from this step*

Numerical Results

- Will use potential-based TDIEs to illustrate the significance of understanding the temporal Sobolev spaces to achieve a stable MOT discretization
- Eigenvalue stability analysis will be performed to rigorously demonstrate stability or instability of a discretization
  - Performed by forming an auxiliary matrix that fully describes the time marching process
  - Eigenvalues of auxiliary matrix are calculated – if any eigenvalues are outside the unit circle the method is unstable
- All results are for a 1 meter radius PEC sphere
- All simulations have been run with every method, but not all results are shown for brevity
  - Results are consistent – if a system is unstable for one simulation it was unstable for all, same with stable systems





Numerical Results

- Equations on this slide are found by taking the inverse Fourier transform of frequency domain potential-based integral equations
  - DOI: 10.1109/TAP.2018.2794388
- These equations have different temporal range spaces
- Naively choosing unknown source functions leads to different temporal domain spaces
  - Unknowns require different temporal basis functions
- No choice of basis functions in MOT discretization will achieve stable results for this system
- Use quadratic B-spline as temporal basis function for both unknowns for these results

Naïve Potential-Based TDIE System

$$\hat{n} \times \int_S \left[\mu \frac{\mathbf{J}(\mathbf{r}', t - R/c)}{4\pi R} - \nabla \frac{\Sigma(\mathbf{r}', t - R/c)}{4\pi R} \right] dS' = \mathbf{A}^{\text{inc}}(\mathbf{r}, t) \times \hat{n}$$

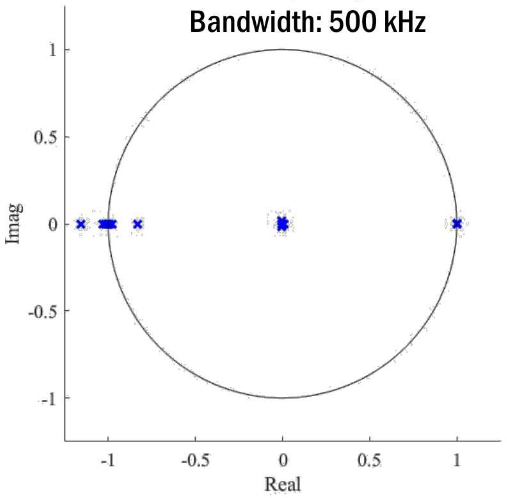
$$\int_S \left[\epsilon^{-1} \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}', t - R/c)}{4\pi R} - \frac{\ddot{\Sigma}(\mathbf{r}', t - R/c)}{4\pi R} \right] dS' = \dot{\Phi}^{\text{inc}}(\mathbf{r}, t)$$

Unknowns: $\mathbf{J}(\mathbf{r}', t), \ \Sigma(\mathbf{r}', t) = \hat{n}' \cdot \mathbf{A}(\mathbf{r}', t)$

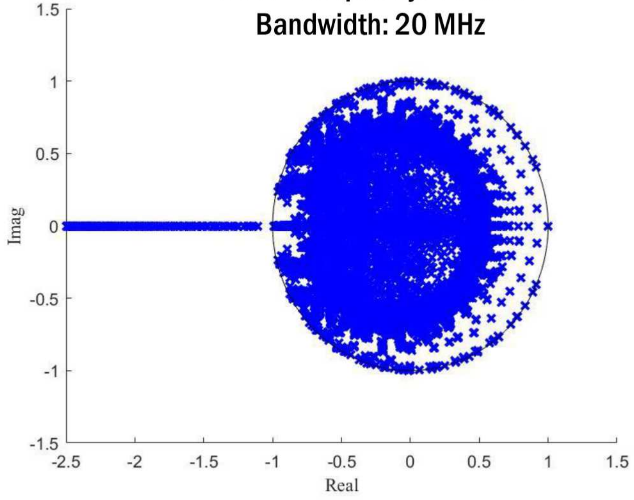
Different temporal range spaces

Different temporal domain spaces

Center Frequency: 1 MHz
Bandwidth: 500 kHz



Center Frequency: 80 MHz
Bandwidth: 20 MHz



Highly unstable system due to inconsistent equations and discretization

Numerical Results:

- Equations on this slide were developed so a stable MOT discretization could be implemented
- Equations have the same temporal range spaces
  - Dirac delta function in the dual to this range space – directly gives MOT method
- Unknown source functions have the same domain space
  - Unknowns can use the same temporal basis functions
- Despite correct equations, if we use a basis function from incorrect domain space the MOT system is unstable
- MOT basis functions:
  - Incorrect: quadratic B-spline
  - Correct: triangle

Differentiated A-Φ Integral Equations (D-APIE)

$$\hat{n} \times \int_S \left[\mu \frac{\dot{\mathbf{J}}(\mathbf{r}', t - R/c)}{4\pi R} - \nabla \frac{\Pi(\mathbf{r}', t - R/c)}{4\pi R} \right] dS' = \dot{\mathbf{A}}^{\text{inc}}(\mathbf{r}, t) \times \hat{n}$$

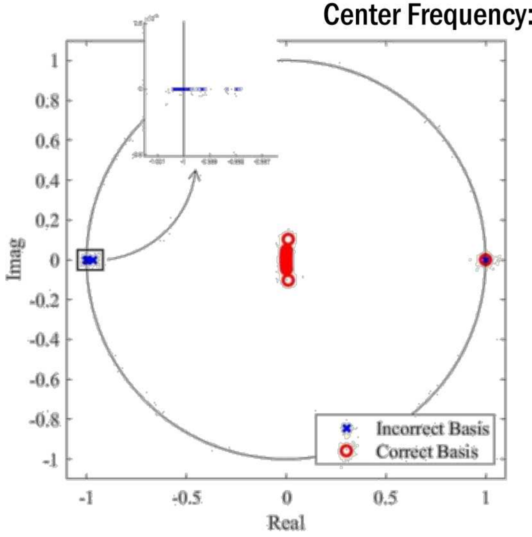
$$\int_S \left[\epsilon^{-1} \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}', t - R/c)}{4\pi R} - \frac{\dot{\Pi}(\mathbf{r}', t - R/c)}{4\pi R} \right] dS' = \dot{\Phi}^{\text{inc}}(\mathbf{r}, t)$$

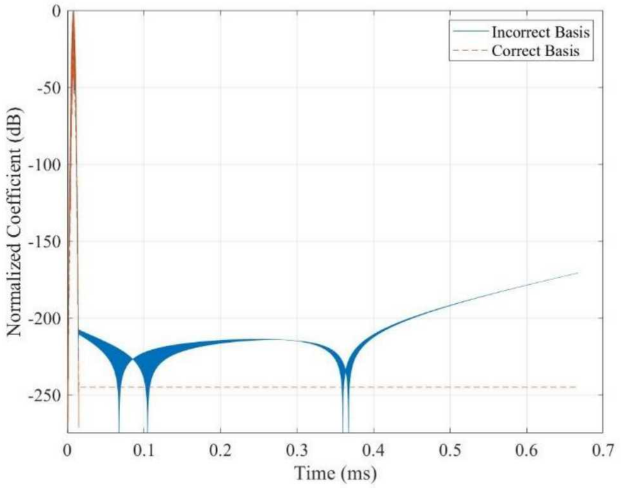
Unknowns: $\mathbf{J}(\mathbf{r}', t), \ \Pi(\mathbf{r}', t) = \hat{n}' \cdot \dot{\mathbf{A}}(\mathbf{r}', t)$

Same temporal range spaces

Same temporal domain spaces

Center Frequency: 1 MHz, Bandwidth: 500 kHz





Improved stability for equations with same range space; basis still must be selected correctly

Numerical Results:

- Equations on this slide were developed to compute potentials directly rather than time derivatives of them
- APIE has a higher order range space than D-APIE
  - Leads to lower order dual space – no longer directly get MOT method
- Can map problem to one with acceptable MOT discretization by choosing basis functions from different domain space
- System will be unstable if this is ignored (essentially using the wrong testing space)
- MOT basis functions:
  - Incorrect: triangle
  - Correct: pulse (constant over 2 time steps)

A-Φ Integral Equations (APIE)

$$\hat{n}\times\int_S\left[\mu\frac{\mathbf{J}(\mathbf{r}',t-R/c)}{4\pi R}-\nabla\int_{-\infty}^{t-R/c}\frac{\Pi(\mathbf{r}',t')}{4\pi R}dt'\right]dS'=\mathbf{A}^{\mathrm{inc}}(\mathbf{r},t)\times\hat{n}$$

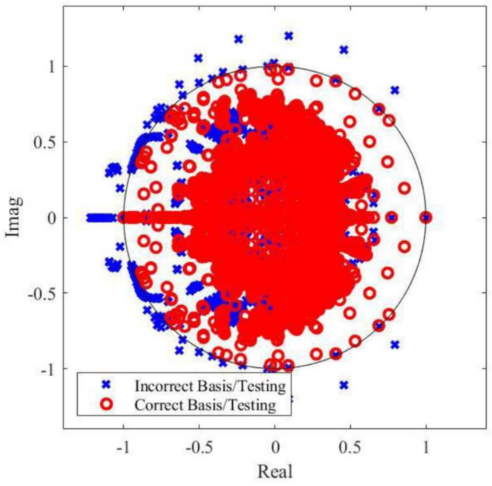
$$\int_S\left[\epsilon^{-1}\int_{-\infty}^{t-R/c}\frac{\nabla'\cdot\mathbf{J}(\mathbf{r}',t')}{4\pi R}dt'-\frac{\Pi(\mathbf{r}',t-R/c)}{4\pi R}\right]dS'=\Phi^{\mathrm{inc}}(\mathbf{r},t)$$

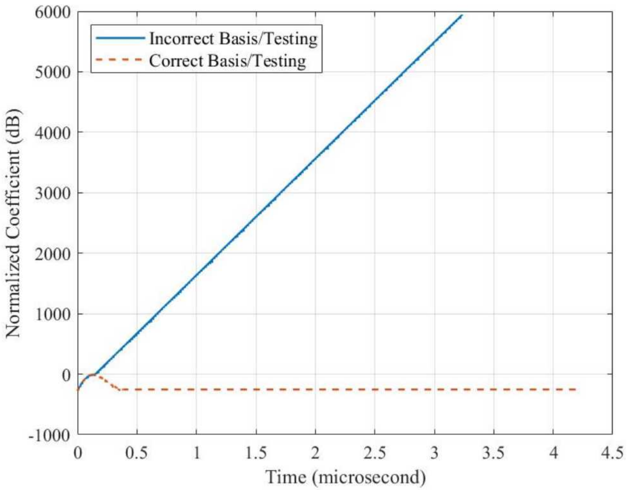
Unknowns: $\mathbf{J}(\mathbf{r}',t),\ \Pi(\mathbf{r}',t)=\hat{n}'\cdot\dot{\mathbf{A}}(\mathbf{r}',t)$

Same temporal range spaces

Same temporal domain spaces

Center Frequency: 30 MHz, Bandwidth: 29 MHz





Acceptable MOT system can be found even if test space doesn't directly give MOT method

Conclusion

- Stability of MOT method depends on much more than just accurately evaluating numerical integrations
- Understanding the spatial and *temporal* Sobolev spaces associated with an integral equation is necessary to develop robustly stable MOT discretizations
  - Domain space helps determine acceptable basis functions
  - Range space helps determine acceptable testing functions (by selecting them from the dual space)
- Although only results for the PEC case were shown, similar effects have been seen with potential-based TDIEs for dielectric regions

Future Work

- Further simplification of functional analysis techniques so they can be more readily utilized by a broader community
- Are there more intuitive, physical explanations underpinning why deviation from the appropriate Sobolev spaces leads to instability?

Acknowledgments

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